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Analysis of vertical cracking phenomena in tensile-strained epitaxial film on a substrate: Part I. Mathematical formulation

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Abstract

This paper presents an analysis of a single vertical crack and periodically distributed vertical cracks in an epitaxial film on a semi-infinite substrate where the cracks penetrate into the substrate. The film and substrate materials have different anisotropic elastic constants, necessitating Stroh formalism in the analysis. The misfit strain due to the lattice mismatch between the film and the substrate serves as the driving force for crack formation. The solution for a dislocation in an anisotropic trimaterial is used as a Green function, so that the cracks are modeled as the continuous distributions of dislocations to yield the singular integral equations of Cauchy-type. The Gauss–Chebyshev quadrature formula is adopted to solve the singular integral equations numerically. Energy arguments provide the critical condition for crack formation, at which the cracks are energetically favorable configurations, in terms of the ratio of the penetration depth into the substrate to the film thickness, the ratio of the spacing of the periodic cracks to the film thickness, and the generalized Dundurs parameters between the film and substrate materials.

Keywords: Anisotropic elasticity; Channeling crack; Vertical crack; Critical condition for crack formation; Continuous distributions of dislocations; Epitaxial film/substrate system

1. Introduction

Presently, strained-layer semiconductor materials are receiving great attention, due to their potential applications in high-speed electronic and optoelectronic devices. Advances in crystal growth techniques,

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e.g., molecular beam epitaxy and organometallic vapor phase epitaxy, make it possible to fabricate highly ordered crystalline structures. At the initial stage of heteroepitaxy, in which the lattice constant of an epitaxial film is usually different from that of a substrate, a misfit strain is developed in the film to maintain the coherency in the atomic arrangements. The misfit strain sometimes has a beneficial effect on the electronic properties of the system, e.g., the bandgap energy (Lee and Park, 2002). However, a principal difficulty with heteroepitaxial layers is that the misfit stress associated with the misfit strain acts as a driving force for structural defects, such as dislocations, islands, surface undulation, composition modulation, cracks, etc., by which the misfit strain is released to minimize the total free energy of the system. Although cracking in a tensile strained epitaxial layer was first reported in 1972 (Matthews and Klokholm, 1972), few studies have investigated the cracking mechanism. Only recently has cracking in III–V epitaxial layers attracted more attention, due to the increasing technological interest in growing highly strained structures (Dieguez et al., 1997; Wu and Weatherly, 1999; Murray et al., 2000; Natali et al., 2000).

Among the many cracking patterns in film/substrate systems as summarized by Hutchinson and Suo (1992) and Freund and Suresh (2003), channeling cracks are frequently observed in tensile strained brittle films. Thouless (1990) obtained the critical condition for simultaneous formation of channeling cracks based on energy balance, which was modified by Thouless et al. (1992) by considering the sequential formation of cracks. Independently, Hutchinson and Suo (1992) obtained slightly different results by considering the sequential formation of periodic cracks. Beuth (1992) and Shenoy et al. (2000) extended the energy argument to take into account the difference of elastic constants between film and substrate. All the foregoing analyses were restricted to isotropic materials; however, the epitaxial film/substrate systems considered in this paper are single crystals and inherently anisotropic. A phenomenon of cracking into substrate is frequently observed in epitaxial film/substrate systems, which has not been extensively studied, except for the analyses of Murray et al. (2000) and Zhang and Zhao (2002). In this paper, vertical cracks, such as those shown in Fig. 1, are analyzed by using two-dimensional anisotropic elasticity, in which the difference of elastic constants between film and substrate materials is taken into account. The solution for a dislocation in an anisotropic trimaterial (Choi and Earmme, 2002) is used as a Green function, so that the cracks are modeled as the continuous distributions of dislocations, which yield the singular integral equations of Cauchy-type. The Gauss–Chebyshev quadrature formula, as summarized by Hills et al. (1996), is adopted to solve the singular integral equations numerically. Thus, the critical condition for the vertical crack formation is obtained. The present analysis scheme might be more suitable in parametric studies on the critical condition for crack formation than the finite element method is. The mathematical formulations to obtain the critical condition for the onset of cracks are delivered in this paper (Part I. Mathematical formulation),

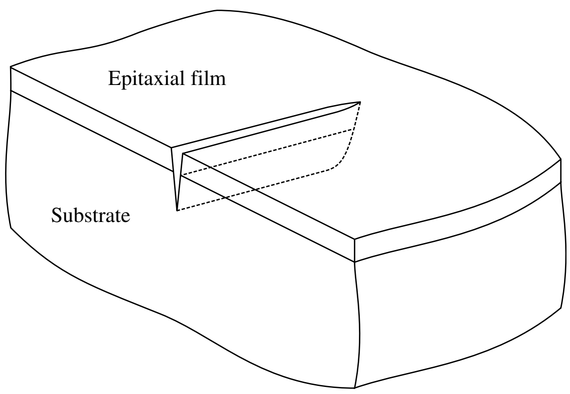

Fig. 1. Typical cracking phenomenon in tensile-strained epitaxial film on a substrate, in which the crack penetrates into the substrate.

while the practical applications and numerical results will be given in a companion paper (Part II. Application to $In_xGa_{1-x}As/InP$ system), the subsequent paper (Lee et al., in preparation).

2. Stroh formalism and Green's functions

2.1. Stroh formalism

We begin with the brief review of anisotropic elasticity by considering a generalized two-dimensional deformation, in which the displacements u_j depend only on x_1 and x_2. The constitutive equations for a linear elastic material are

$$\sigma_{ij} = C_{ijkm}\frac{\partial u_k}{\partial x_m}, \quad (i, j = 1, 2, 3) \tag{1}$$

in which σ_{ij} are the stresses and C_{ijkm} are the elastic constants. Throughout this paper, the convention of summation *over repeated Latin subscripts* is used, while summation *over repeated Greek subscripts* will always be indicated explicitly. The equations of equilibrium are

$$C_{ijkm}\frac{\partial^2 u_k}{\partial x_j \partial x_m} = 0. \tag{2}$$

A general solution for the displacements satisfying Eq. (2) and the corresponding stresses may be written as follows (Eshelby et al., 1953; Stroh, 1958):

$$u_i = 2\mathrm{Re}\left[\sum_{\alpha=1}^{3} A_{i\alpha} f_\alpha(z_\alpha)\right], \tag{3}$$

$$\sigma_{1i} = -2\mathrm{Re}\left[\sum_{\alpha=1}^{3} B_{i\alpha} p_\alpha f'_\alpha(z_\alpha)\right], \tag{4}$$

$$\sigma_{2i} = 2\mathrm{Re}\left[\sum_{\alpha=1}^{3} B_{i\alpha} f'_\alpha(z_\alpha)\right]. \tag{5}$$

Here the prime implies the derivative with respect to the associated argument. The functions $f_j(z_j)$ are analytic functions of complex variable $z_j = x_1 + p_j x_2$. Each column of $\mathbf{A}$ and each of p_j's are the eigenvector and the eigenvalue with positive imaginary part, respectively, of the sextic equation

$$[C_{1i1j} + (C_{1i2j} + C_{2i1j})p_\alpha + C_{2i2j}p_\alpha^2]A_{j\alpha} = 0. \tag{6}$$

The matrix $\mathbf{B}$ is given by

$$B_{i\alpha} = (C_{i2j1} + p_\alpha C_{i2j2})A_{j\alpha}. \tag{7}$$

If Eq. (6) has three distinct pairs of complex roots on which we are concentrating, the matrices $\mathbf{A}$ and $\mathbf{B}$ are non-singular and may be used to define

$$\mathbf{M}^{-1} \equiv \mathrm{i}\mathbf{A}\mathbf{B}^{-1}, \tag{8}$$

which is a positive-definite Hermitian matrix (Stroh, 1958). Here, $\mathrm{i} = \sqrt{-1}$ and $(\,)^{-1}$ stands for the inverse of a matrix. Explicit expressions of $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{M}^{-1}$ in terms of elastic constants are given in Suo (1990) and Ting (1996). The symbols $\mathbf{L}$ and $\mathbf{B}$ used in Suo's paper correspond to $\mathbf{B}$ and $\mathbf{M}^{-1}$ in this paper, respectively. For mathematical simplicity, we introduce three more bimaterial matrices, as follows (Choi and Earmme, 2002):

$$\mathbf{T}^{ab} \equiv \left[(\mathbf{M}^a)^{-1} + (\overline{\mathbf{M}}^b)^{-1}\right]^{-1}\left[(\mathbf{M}^b)^{-1} - (\mathbf{M}^a)^{-1}\right], \tag{9}$$

$$\mathbf{U}^{ab} = (\mathbf{B}^a)^{-1}(\mathbf{I} + \mathbf{T}^{ab})\mathbf{B}^b, \tag{10}$$

$$\mathbf{V}^{ab} = (\overline{\mathbf{B}}^b)^{-1}\mathbf{T}^{ab}\mathbf{B}^b. \tag{11}$$

In the foregoing bimaterial matrices, the overbar denotes the complex conjugate, and the superscripts a and b refer to materials a and b, respectively.

2.2. Green's functions for a dislocation in an anisotropic film/substrate structure

Using the method of analytic continuation and Schwarz–Neumann's alternating technique, Choi and Earmme (2002) obtained a solution for a singularity such as a dislocation or a line force in an anisotropic 'trimaterial', which denotes an infinite body composed of three dissimilar materials bonded along two parallel interfaces. When the outer one of the three constituent materials is absent, their solution for a singularity in an anisotropic trimaterial is still valid; therefore, the solution for a singularity in a film/substrate structure can be easily obtained, and it serves as the Green function for solving the crack problems in Section 3. Here we summarize the essential parts of the results of Choi and Earmme (2002) to proceed.

The analytic function $f^0_{\alpha k}(z)$ for a dislocation having a unit Burgers vector in the direction of $\boldsymbol{e}_k$ at (x^0_1, x^0_2) in an infinite homogeneous medium is used as a basis for the corresponding solution for the dislocation in a trimaterial, given as (Stroh, 1958; Suo, 1990)

$$f^0_{\alpha k}(z) = q_{\alpha k}\ln(z - s_\alpha), \tag{12}$$

where $s_\alpha = x^0_1 + p_\alpha x^0_2$ and $\mathbf{q}_k \equiv \{q_{\alpha k}\} = (1/2\pi)\mathbf{B}^{-1}(\mathbf{M}^{-1} + \overline{\mathbf{M}}^{-1})^{-1}\boldsymbol{e}_k$. Similarly, the solution for a periodic array of identical dislocations in an infinite homogeneous medium becomes a basis to build the corresponding solution for the periodic array of identical dislocations in a trimaterial. With the solution for a dislocation, Eq. (12), the solution for a periodic array of identical dislocations can be found by superposition. Let λ be the spacing between dislocations. The analytic functions for dislocations located at $(x^0_1 + n\lambda, x^0_2)$ are simply summed for $n = \ldots, -2, -1, 0, 1, 2, \ldots$, leading to

$$f^0_{\alpha k}(z) = q_{\alpha k}\ln\left\{\sin\left[\frac{\pi}{\lambda}(z - s_\alpha)\right]\right\}. \tag{13}$$

Here all the dislocations in the periodic array have a unit Burgers vector in the direction of $\boldsymbol{e}_k$.

Next, consider an anisotropic film of thickness h on a semi-infinite anisotropic substrate, such as that shown in Fig. 2(a) though without a crack. If a dislocation is located at (x^0_1, x^0_2) in the film, the $(1, i)$ components of the stress tensor in the film and substrate are given as (Choi and Earmme, 2002)

$$G^{ff}_{1ik}(x_1, x_2; x^0_1, x^0_2) = -2\mathrm{Re}\left\{\sum_{n=1}^{\infty}\left[\sum_{\alpha=1}^{3} B^f_{i\alpha}p^f_\alpha f^{n\prime}_{\alpha k}(z^f_\alpha) + \sum_{\alpha,\beta=1}^{3} B^f_{i\alpha}p^f_\alpha \overline{V}^{ef}_{\alpha\beta}\bar{f}^{n\prime}_{\beta k}(z^f_\alpha - p^f_\alpha h + \bar{p}^f_\beta h)\right]\right\} \tag{14a}$$

and

$$G^{sf}_{1ik}(x_1, x_2; x^0_1, x^0_2) = -2\mathrm{Re}\left\{\sum_{\alpha,\beta=1}^{3} B^s_{i\alpha}p^s_\alpha U^{sf}_{\alpha\beta}f^{0\prime}_{\beta k}(z^s_\alpha) + \sum_{\alpha,\beta,\gamma=1}^{3} B^s_{i\alpha}p^s_\alpha U^{sf}_{\alpha\beta}\overline{V}^{ef}_{\beta\gamma}\left[\sum_{n=1}^{\infty}\bar{f}^{n\prime}_{\gamma k}(z^s_\alpha - p^f_\beta h + \bar{p}^f_\gamma h)\right]\right\}, \tag{14b}$$

respectively; in these equations, the superscripts e, f, and s refer to the empty region, the film, and the substrate, respectively, and the Green function $G^{ab}_{ijk}(x_1, x_2; x^0_1, x^0_2)$ denotes the (i, j) component of the stress tensor at (x_1, x_2) in material a due to a dislocation of unit Burgers vector in the direction of $\boldsymbol{e}_k$ located at (x^0_1, x^0_2) in material b. The recurrence formula for $f^n_{\alpha k}(z)$ is given by

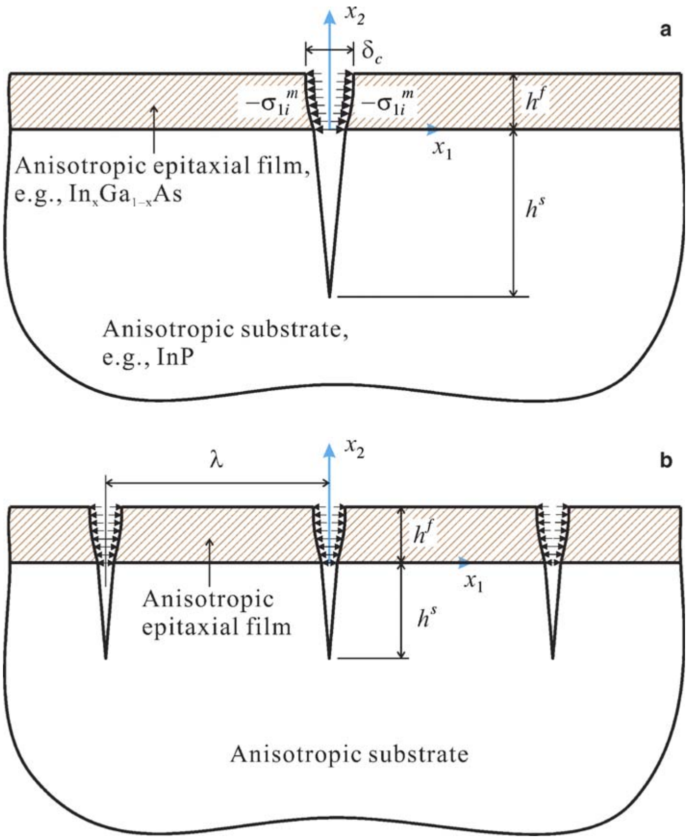

Fig. 2. Schematic diagrams of the channeling crack problems in an epitaxial film on a substrate: (a) a single vertical crack and (b) periodically distributed vertical cracks.

$$f_{\alpha k}^{n+1}(z) = \begin{cases} f_{\alpha k}^{0}(z) + \sum\limits_{\beta=1}^{3} \overline{V}_{\alpha\beta}^{sf} \bar{f}_{\beta k}^{0}(z), & \text{if } n = 0, \\ \sum\limits_{\beta,\gamma=1}^{3} \overline{V}_{\alpha\beta}^{ef} V_{\beta\gamma}^{ef} f_{\gamma k}^{n}(z - \bar{p}_{\beta}^{f} h + p_{\gamma}^{f} h), & \text{if } n = 1, 2, 3, \ldots \end{cases} \tag{15}$$

Here the elastic constants of the film are implied in $f_{\alpha k}^{0}(z)$. If a dislocation is located at (x_1^0, x_2^0) in the substrate, the $(1, i)$ components of the stress tensor in the film and substrate are given as (Choi and Earmme, 2002)

$$G_{1ik}^{fs}(x_1, x_2; x_1^0, x_2^0) = -2\mathrm{Re}\left\{ \sum_{n=1}^{\infty} \left[\sum_{\alpha=1}^{3} B_{i\alpha}^{f} p_{\alpha}^{f} f_{\alpha k}^{n\prime}(z_{\alpha}^{f}) + \sum_{\alpha,\beta=1}^{3} B_{i\alpha}^{f} p_{\alpha}^{f} \overline{V}_{\alpha\beta}^{ef} \bar{f}_{\beta k}^{n\prime}(z_{\alpha}^{f} - p_{\alpha}^{f} h + \bar{p}_{\beta}^{f} h) \right] \right\} \tag{16a}$$

and

$$G_{1ik}^{ss}(x_1, x_2; x_1^0, x_2^0) = -2\mathrm{Re}\left\{ \sum_{\alpha=1}^{3} B_{i\alpha}^{s} p_{\alpha}^{s} f_{\alpha k}^{0\prime}(z_{\alpha}^{s}) + \sum_{\alpha,\beta=1}^{3} B_{i\alpha}^{s} p_{\alpha}^{s} \overline{V}_{\alpha\beta}^{fs} \bar{f}_{\beta k}^{0\prime}(z_{\alpha}^{s}) + \sum_{\alpha,\beta,\gamma=1}^{3} B_{i\alpha}^{s} p_{\alpha}^{s} U_{\alpha\beta}^{sf} \overline{V}_{\beta\gamma}^{ef} \left[\sum_{n=1}^{\infty} \bar{f}_{\gamma k}^{n\prime}(z_{\alpha}^{s} - p_{\beta}^{f} h + \bar{p}_{\gamma}^{f} h) \right] \right\}, \tag{16b}$$

respectively, and the recurrence formula for $f^n_{\alpha k}(z)$ is given by

$$f^{n+1}_{\alpha k}(z) = \begin{cases} \sum\limits_{\beta=1}^{3} U^{fs}_{\alpha\beta} f^0_{\beta k}(z), & \text{if } n = 0, \\ \sum\limits_{\beta,\gamma=1}^{3} \overline{V}^{sf}_{\alpha\beta} V^{ef}_{\beta\gamma} f^n_{\gamma k}(z - \bar{p}^f_\beta h + p^f_\gamma h), & \text{if } n = 1, 2, 3, \ldots \end{cases} \tag{17}$$

Here the elastic constants of the substrate are implied in $f^0_{\alpha k}(z)$. It should be noted that even if a periodic array of identical dislocations, rather than a single dislocation, is located in a film/substrate structure, Eqs. (14)–(17) are still valid provided that the corresponding homogeneous solution given in Eq. (13) instead of that in Eq. (12) is used in Eqs. (14)–(17).

3. Cracking problem and mathematical formulation

3.1. Problem definition

Consider an epitaxial film of thickness h^f on a semi-infinite substrate, as shown in Fig. 2(a). Both the film and substrate materials are anisotropic solids, having the x_1x_2 plane as a mirror plane so that the plane deformation with respect to the x_1x_2 plane is assumed. In addition, the film material is assumed to have cubic symmetry, as do most III–V compound semiconductor materials. The anisotropic misfit strains have been defined in Zhang (1995) as

$$\varepsilon^m_{ij} = \frac{1}{2}\left[\frac{\sum_{\alpha=1}^{3}(a^s_{\alpha i} - a^f_{\alpha i})}{\sum_{\alpha=1}^{3} a^f_{\alpha j}} + \frac{\sum_{\alpha=1}^{3}(a^s_{\alpha j} - a^f_{\alpha j})}{\sum_{\alpha=1}^{3} a^f_{\alpha i}}\right], \tag{18}$$

where $a^f_{\alpha i}$ and $a^s_{\alpha i}$ are the i components of the αth primitive lattice vectors of the epitaxial film and the substrate, respectively. For the cubic symmetry, Eq. (18) is reduced to

$$\varepsilon^m_{ij} = \frac{a^s - a^f}{a^f}\delta_{ij}, \tag{19}$$

where δ_{ij} is the Kronecker delta. Hence, the corresponding misfit stress is given by (Gosling and Willis, 1994)

$$\sigma^m_{ij} = -(C^f_{ijpq} - C^f_{ijr2}\chi^{-1}_{rs}C^f_{s2pq})\varepsilon^m_{pq}, \quad \chi_{rs} = C^f_{r22s}. \tag{20}$$

Thermal stresses, due to the mismatch of thermal expansion coefficients developed while growing the film, are not considered here; however, if necessary, thermal stresses can be included in the analysis without difficulty.

For certain combinations of the film and substrate materials, for example, an $In_xGa_{1-x}As$ ($x = 0.25$) film on an InP substrate, relaxation of the misfit strain energy stored in the film generates vertical cracks in the film that penetrate into the substrate (Wu and Weatherly, 1999). If the crack length within the substrate is h^s, as shown in Fig. 2(a), then the total length of the vertical crack is $h^f + h^s$. Fig. 2(a) shows a single vertical crack, while a periodic array of vertical cracks is schematically drawn in Fig. 2(b) that illustrates a common situation in the growth of epitaxial films. The crack surfaces within the film have a crack-face loading equal to $-\sigma^m_{1i}$. The stress fields caused by crack-face loading, as shown in Fig. 2, are solved and then superposed with the uniform stress fields, given as Eq. (20), due to the misfit strain. Then we can obtain a solution for vertical cracking due to the lattice mismatch in the epitaxial film/substrate structures (Fig. 1), where all the crack surfaces become traction-free. In this study, a single crack (Fig. 2(a)) and a periodic array of cracks

(Fig. 2(b)) are analyzed by using the Green functions for a dislocation in a trimaterial and for the continuous distribution of dislocations.

3.2. Formulation of singular integral equations

Using the method of analytic continuation and Schwarz–Neumann's alternating technique, Choi and Earmme (2002) obtained the solution for a dislocation in an anisotropic trimaterial. The Green functions for a dislocation in a film/substrate structure are summarized in Section 2.2. The Green function $G^{ab}_{ijk}(x_1,x_2;x_1^0,x_2^0)$ denotes the (i,j) component of the stress tensor at (x_1,x_2) in material a due to a dislocation of unit Burgers vector in the direction of $\boldsymbol{e}_k$ located at (x_1^0,x_2^0) in material b. As noted in Section 2.2, the Green functions for a periodic array of identical dislocations in a film/substrate structure have the same forms, except that the corresponding homogeneous solution for a dislocation, Eq. (12), is replaced by Eq. (13), which is the homogeneous solution for a periodic array of identical dislocations. Therefore, we can use the same Green function $G^{ab}_{ijk}(x_1,x_2;x_1^0,x_2^0)$ both for a single dislocation and for a periodic array of identical dislocations. Furthermore, the solution procedure for periodically distributed cracks, as depicted in Fig. 2(b), must be identical to that for a single crack, as depicted in Fig. 2(a). In the following analysis, we deal with a single crack problem, and the same formulation can be used straightforwardly for a periodic array of vertical cracks.

Let us return to the crack problem illustrated in Fig. 2(a), which can be solved via the continuous dislocations distributed along the crack surface, i.e., $x_1=0$, $-h^s<x_2<h^f$. The boundary conditions on the crack surfaces are reduced to the following relations:

$$\sigma^{ff}_{1i}(0,x_2)+\sigma^{fs}_{1i}(0,x_2)=\sigma^{m}_{1i},\quad (i=1,2,3;\ 0\leqslant x_2\leqslant h^f),\tag{21a}$$

$$\sigma^{sf}_{1i}(0,x_2)+\sigma^{ss}_{1i}(0,x_2)=0,\quad (i=1,2,3;\ -h^s\leqslant x_2\leqslant 0)\tag{21b}$$

in which $\sigma^{ab}_{ij}(x_1,x_2)$ represents the (i,j) component of the stress tensor at (x_1,x_2) in material a due to the continuous distribution of dislocations in material b. Using the Green functions for a dislocation in the film/substrate structure given in Section 2.2, Eqs. (21a) and (21b) can be rewritten as

$$\int_0^{h^f} G^{ff}_{1ik}(0,x_2;0,s)\psi^f_k(s)\,\mathrm{d}s+\int_{-h^s}^{0} G^{fs}_{1ik}(0,x_2;0,s)\psi^s_k(s)\,\mathrm{d}s=\sigma^m_{1i},\quad (i=1,2,3;\ 0\leqslant x_2\leqslant h^f)\tag{22a}$$

$$\int_0^{h^f} G^{sf}_{1ik}(0,x_2;0,s)\psi^f_k(s)\,\mathrm{d}s+\int_{-h^s}^{0} G^{ss}_{1ik}(0,x_2;0,s)\psi^s_k(s)\,\mathrm{d}s=0,\quad (i=1,2,3;\ -h^s\leqslant x_2\leqslant 0)\tag{22b}$$

in which $\psi^f(s)(=\{\psi^f_1(s),\psi^f_2(s),\psi^f_3(s)\})$ and $\psi^s(s)(=\{\psi^s_1(s),\psi^s_2(s),\psi^s_3(s)\})$ are the dislocation density functions in the film and in the substrate, respectively. Eqs. (22a) and (22b) are the system of singular integral equations of Cauchy type, which can be numerically solved. To use Gauss–Chebyshev quadrature formulae, Eqs. (22a) and (22b) are normalized so that the integration domains are converted to the standard interval $[-1,1]$, resulting in

$$h^f\int_{-1}^{1}\Gamma^{ff}_{1ik}(\tilde t,\tilde s)\zeta^f_k(\tilde s)\,\mathrm{d}\tilde s+h^s\int_{-1}^{1}\Gamma^{fs}_{1ik}(\tilde t,\hat s)\zeta^s_k(\hat s)\,\mathrm{d}\hat s=2\sigma^m_{1i}\quad (i=1,2,3;\ -1\leqslant\tilde t\leqslant 1),\tag{23a}$$

$$h^f\int_{-1}^{1}\Gamma^{sf}_{1ik}(\hat t,\tilde s)\zeta^f_k(\tilde s)\,\mathrm{d}\tilde s+h^s\int_{-1}^{1}\Gamma^{ss}_{1ik}(\hat t,\hat s)\zeta^s_k(\hat s)\,\mathrm{d}\hat s=0\quad (i=1,2,3;\ -1\leqslant\hat t\leqslant 1)\tag{23b}$$

in which the length variables with the tilde ($\sim$) are the variables normalized by the relation $\tilde s=2s/h^f-1$, and those with the hat ($\wedge$) are the variables normalized by the rule $\hat s=2s/h^s+1$. The new Green functions and dislocation density functions in Eqs. (23a) and (23b) are defined so that their arguments are expressed in terms of the appropriate normalized variables, for example, $\Gamma^{fs}_{1ik}(\tilde{t},\hat{s}) \equiv G^{fs}_{1ik}[0,(\tilde{t}+1)h^f/2;0,(\hat{s}-1)h^s/2]$ and $\zeta^s_k(\hat{s}) \equiv \psi^s_k[(\hat{s}-1)h^s/2]$.

4. Numerical calculation and energy release rate

To solve the system of singular integral equations given in Eqs. (23a) and (23b), Gauss–Chebyshev quadrature formulae are utilized; thus, the formulae for the stress intensity factors and the energy release rate are expressed in terms of the dislocation density functions.

4.1. Discretization of singular integral equations

We begin by considering the singular behavior of the dislocation density functions. When we model a crack as a continuous distribution of infinitesimal dislocations, a dislocation density function at a point physically represents the magnitude of the slope of the crack surface shape at the point along the crack faces. Near the crack-tip in the substrate, the dislocation density tends to infinity in a square-root-singular manner, while the dislocation density is bounded near the edge where the crack meets the free surface. When the straight crack crosses the film/substrate interface, the dislocation density near the interface has a singular behavior weaker than the square-root singularity. Therefore, the dislocation density functions may be written as follows:

$$\boldsymbol{\zeta}^f(\tilde{s}) = \omega^f(\tilde{s})\boldsymbol{\Phi}^f(\tilde{s}), \quad \omega^f(\tilde{s}) = (1-\tilde{s})^{1/2}(1+\tilde{s})^{\kappa}, \tag{24a}$$

$$\boldsymbol{\zeta}^s(\hat{s}) = \omega^s(\hat{s})\boldsymbol{\Phi}^s(\hat{s}), \quad \omega^s(\hat{s}) = (1-\hat{s})^{\kappa'}(1+\hat{s})^{-1/2}. \tag{24b}$$

Here κ and κ' are the eigenvalues of characteristic equations depending on the material properties as well as the wedge geometry and provide weak singularities, that is, $-1/2 < \kappa,\ \kappa' < 0$. $\boldsymbol{\Phi}^f(\tilde{s})$ and $\boldsymbol{\Phi}^s(\hat{s})$ are bounded functions, and $\omega^f(\tilde{s})$ and $\omega^s(\hat{s})$ are called weight functions. We cannot use the Gauss–Chebyshev quadrature directly, because it is of use only for weight functions having powers of $\pm 1/2$. Instead, we adopt the procedure developed by Sheng and Wheeler (1981), which is appropriate for our analysis, since the primary concern is the behavior of the dislocation densities at the crack tip, rather than an evaluation of quantities very close to the interface. First, we assume an over-severe singularity, i.e., the square-root singularity, at the interface so that

$$\boldsymbol{\zeta}^f(\tilde{s}) = \sqrt{\frac{1-\tilde{s}}{1+\tilde{s}}}\boldsymbol{\varphi}^f(\tilde{s}), \tag{25a}$$

$$\boldsymbol{\zeta}^s(\hat{s}) = \frac{1}{\sqrt{1-\hat{s}^2}}\boldsymbol{\varphi}^s(\hat{s}), \tag{25b}$$

in which $\boldsymbol{\varphi}^f(\tilde{s}) = \boldsymbol{\Phi}^f(\tilde{s})(1+\tilde{s})^{\kappa+1/2}$ and $\boldsymbol{\varphi}^s(\hat{s}) = \boldsymbol{\Phi}^s(\hat{s})(1-\hat{s})^{\kappa'+1/2}$. It is worth noting that since $\kappa+1/2$ and $\kappa'+1/2$ are always positive, $\boldsymbol{\varphi}^f(\tilde{s})$ and $\boldsymbol{\varphi}^s(\hat{s})$ are bounded functions, and at the interface

$$\boldsymbol{\varphi}^f(-1) = \mathbf{0}, \tag{26a}$$

$$\boldsymbol{\varphi}^s(+1) = \mathbf{0}. \tag{26b}$$

Either one of Eq. (26a) or Eq. (26b) can be used as an additional condition for the dislocation density functions.

The singular integral equations given in Eqs. (23a) and (23b) with Eqs. (25a) and (25b) may be reduced to a set of algebraic equations by applying the Gauss–Chebyshev quadrature formula, of which the standard procedure is well summarized by Hills et al. (1996), resulting in

$$\frac{2\pi h^f}{2N+1}\sum_{n=1}^{N}(1-\tilde{s}_n)\Gamma^{ff}_{1ik}(\tilde{t}_m,\tilde{s}_n)\varphi^f_k(\tilde{s}_n)+\frac{\pi h^s}{N}\sum_{n=1}^{N}\Gamma^{fs}_{1ik}(\tilde{t}_m,\hat{s}_n)\varphi^s_k(\hat{s}_n)=2\sigma^m_{1i}\quad (m=1,2,\ldots,N), \tag{27a}$$

$$\frac{2\pi h^f}{2N+1}\sum_{n=1}^{N}(1-\tilde{s}_n)\Gamma^{sf}_{1ik}(\hat{t}_m,\tilde{s}_n)\varphi^f_k(\tilde{s}_n)+\frac{\pi h^s}{N}\sum_{n=1}^{N}\Gamma^{ss}_{1ik}(\hat{t}_m,\hat{s}_n)\varphi^s_k(\hat{s}_n)=0\quad (m=1,2,\ldots,N-1). \tag{27b}$$

Here the integration points, $\tilde{s}_n$ and $\hat{s}_n$, and the collocation points, $\tilde{t}_m$ and $\hat{t}_m$, are given by (Hills et al., 1996)

$$\tilde{s}_n=\cos\left(\pi\frac{2n}{2N+1}\right),\quad \hat{s}_n=\cos\left(\pi\frac{2n-1}{2N}\right), \tag{28a}$$

$$\tilde{t}_m=\cos\left(\pi\frac{2m-1}{2N+1}\right),\quad \hat{t}_m=\cos\left(\pi\frac{m}{N}\right), \tag{28b}$$

where N is the number of integration or collocation points. To obtain an additional relation using Eq. (26), we employ Krenk's interpolation formulae (Krenk, 1975), which yield

$$\varphi^f_k(-1)=\frac{2}{2N+1}\sum_{n=1}^{N}\cot\left(\frac{2n-1}{2N+1}\frac{\pi}{2}\right)\sin\left(\frac{2n-1}{2N+1}N\pi\right)\varphi^f_k(\tilde{s}_{N+1-n})=0, \tag{29}$$

or

$$\varphi^s_k(1)=\frac{1}{N}\sum_{n=1}^{N}\left\{\sin\left[\frac{2n-1}{4N}\pi(2N-1)\right]\Big/\sin\left(\frac{2n-1}{4N}\pi\right)\right\}\varphi^s_k(\hat{s}_n)=0. \tag{30}$$

Therefore, Eqs. (27a) and (27b) with either Eq. (29) or Eq. (30) becomes a set of $6N$ algebraic equations in the $6N$ unknowns $\varphi^f_k(\tilde{s}_n)$ and $\varphi^s_k(\hat{s}_n)$ $(k=1,2,3;\ n=1,2,\ldots,N)$, which can be numerically solved.

4.2. Crack opening displacements, stress intensity factors, and energy release rate

Provided that we know the dislocation density $\varphi^f_k(\tilde{s}_n)$ and $\varphi^s_k(\hat{s}_n)$ at N discrete collocation points by solving Eqs. (27a) and (27b) with either Eq. (29) or Eq. (30), Krenk's interpolation formula (Krenk, 1975) can be used to obtain the dislocation density functions at any point on the crack faces as

$$\varphi^f_k(\tilde{s})=\frac{4}{2N+1}\sum_{n=1}^{N}\left\{\sum_{m=0}^{N-1}\sin\left(\frac{n\pi}{2N+1}\right)\sin\left[\frac{n\pi(2m+1)}{2N+1}\right]\frac{\sin[(2m+1)\gamma]}{\sin\gamma}\right\}\varphi^f_k(\tilde{s}_n), \tag{31a}$$

$$\varphi^s_k(\hat{s})=\frac{2}{N}\sum_{n=1}^{N}\left[\frac{1}{2}+\sum_{m=1}^{N-1}\cos\left(\frac{2n-1}{2N}m\pi\right)\cos(m\cos^{-1}\hat{s})\right]\varphi^s_k(\hat{s}_n), \tag{31b}$$

in which $\gamma=\cos^{-1}[\sqrt{(1+\tilde{s})/2}]$. Using the fact that the dislocation density at any point physically represents the slope of the crack surface shape at the point, we can obtain the crack opening displacements by integrating the dislocation density functions given in Eqs. (31a) and (31b).

We can easily obtain the stress intensity factors and energy release rate by comparing the dislocation density $\varphi^f_k(\tilde{s}_n)$ and $\varphi^s_k(\hat{s}_n)$ at N discrete collocation points with the gradient of the crack opening displacement due to asymptotic K-fields. In linear elastic fracture mechanics, the displacements are expressed as (Beom and Atluri, 1996)

$$u_i(x_1,x_2)=\sqrt{\frac{2}{\pi}}\mathrm{Re}\left[\sum_{\alpha=1}^{3}A_{i\alpha}B^{-1}_{\alpha j}k_j\sqrt{z_\alpha}\right]. \tag{32}$$

where $\boldsymbol{k} \equiv (K_{\mathrm{II}}, K_{\mathrm{I}}, K_{\mathrm{III}})$, in which K_{I}, K_{II}, and K_{III} are the mode I, II, and III stress intensity factors, respectively. Then, the crack opening displacements $\boldsymbol{\delta}(x_2)$ are given by

$$\boldsymbol{\delta}(x_2) = \boldsymbol{u}^+(x_2) - \boldsymbol{u}^-(x_2) = 2\sqrt{\frac{2(x_2 + h^s)}{\pi}}(\mathbf{L}^s)^{-1}\boldsymbol{k}, \tag{33}$$

where $(\mathbf{L}^s)^{-1} = \mathrm{Re}[(\mathbf{M}^s)^{-1}]$. Therefore, we may define the stress intensity factors in terms of the gradient of the crack opening displacements as

$$\boldsymbol{k} \equiv \lim_{x_2 \to -h^s} \sqrt{\frac{\pi(x_2 + h^s)}{2}}\mathbf{L}^s \frac{\mathrm{d}\boldsymbol{\delta}(x_2)}{\mathrm{d}x_2}. \tag{34}$$

Recalling that a dislocation density function at any point physically represents the magnitude of the slope of the crack surface shape at the point along the crack faces, and using Eqs. (25b) and (34), we can express the stress intensity factors as

$$\boldsymbol{k} = \sqrt{\frac{\pi h^s}{8}}\mathbf{L}^s \boldsymbol{\varphi}^s(-1), \tag{35}$$

where $\boldsymbol{\varphi}^s(-1)$ can be interpolated in terms of the dislocation densities at the collocation points (Krenk, 1975), yielding

$$\boldsymbol{\varphi}^s(-1) = \frac{1}{N}\sum_{n=1}^{N}\left\{\sin\left[\frac{2n-1}{4N}\pi(2N-1)\right]\Big/\sin\left[\frac{2n-1}{4N}\pi\right]\right\}\boldsymbol{\varphi}^s(\hat{s}_{N+1-n}). \tag{36}$$

The energy release rate for the crack propagation is related to the stress intensity factors as (Beom and Atluri, 1996)

$$\mathscr{G} = \frac{1}{2}\boldsymbol{k}^T(\mathbf{L}^s)^{-1}\boldsymbol{k}. \tag{37}$$

5. Critical condition for crack formation

Without any strain relaxation, the misfit strain energy per unit interface area stored in an epitaxial film amounts to

$$\mathscr{E}^m = \frac{1}{2}\sigma_{ij}^m \varepsilon_{ij}^m h^f. \tag{38}$$

The strain energy $\mathscr{E}^m$ due to the lattice mismatch may be released by the formation of vertical cracks. In this section, we explore the critical condition for the onset of cracking based on the energy balance (Thouless, 1990; Shenoy et al., 2000).

5.1. Critical condition for a single crack formation

When a single vertical crack forms in the film/substrate structure, as shown in Fig. 2(a), the elastic energy per unit length released by the crack formation is given in terms of the crack opening displacements $\boldsymbol{\delta}(x_2)$ as

$$\Delta E^{el} = \frac{1}{2}\sigma_{1i}^m \int_0^{h^f} \delta_i(x_2)\,\mathrm{d}x_2. \tag{39}$$

A dimensional analysis allows us to rewrite Eq. (39) as

$$\Delta E^{el} = \frac{(\sigma_{11}^m h^f)^2}{2C_{1111}^s} \mathscr{G}_*^{sc}\left(\frac{h^s}{h^f}; \boldsymbol{\alpha}, \boldsymbol{\beta}\right). \tag{40}$$

Here $\mathscr{G}_*^{sc}$ is the non-dimensionalized energy release rate for a single crack, and $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are generalized Dundurs parameters for dissimilar anisotropic materials defined as follows (Beom and Atluri, 1995; Ting, 1995):

$$\boldsymbol{\alpha} = (\mathbf{L}^f - \mathbf{L}^s)(\mathbf{L}^f + \mathbf{L}^s)^{-1}, \quad \boldsymbol{\beta} = [(\mathbf{L}^f)^{-1} + (\mathbf{L}^s)^{-1}]^{-1}(\mathbf{W}^f - \mathbf{W}^s), \tag{41}$$

in which $\mathbf{L}^{-1} = \mathrm{Re}[\mathbf{M}^{-1}]$ and $\mathbf{W} = -\mathrm{Im}[\mathbf{M}^{-1}]$.

On the other hand, the consumed energy in the cracking process is related to the fracture energies of the film and the substrate, $\mathscr{F}^f$ and $\mathscr{F}^s$, respectively, by

$$\Delta E^{fr} = \mathscr{F}^f h^f + \mathscr{F}^s h^s. \tag{42}$$

It is assumed in the above equation that when a crack propagates across the interface, there is no effect of the interfacial energy on the crack advance. This is a reasonable assumption for cracking in epitaxial film/substrate systems, in which the film is coherently bonded to the substrate and cracks may propagate along common cleavage planes. For purely elastic fracture processes, the fracture energy is entirely converted into the creating energy of new surfaces; therefore, we may regard the fracture energies $\mathscr{F}^f$ and $\mathscr{F}^s$ as twice the surface energies of the film and the substrate, respectively.

The total change in the energy is expressed by

$$\Delta E = -\Delta E^{el} + \Delta E^{fr}. \tag{43}$$

Substituting Eqs. (40) and (42) into Eq. (43) yields

$$\Delta E = \frac{(\sigma_{11}^m h^f)^2}{2C_{1111}^s}\left[\mathscr{F}_*^f + \mathscr{F}_*^s \frac{h^s}{h^f} - \mathscr{G}_*^{sc}\left(\frac{h^s}{h^f}; \boldsymbol{\alpha}, \boldsymbol{\beta}\right)\right], \tag{44}$$

in which the non-dimensionalized fracture energies $\mathscr{F}_*^f$ and $\mathscr{F}_*^s$ are given by

$$\mathscr{F}_*^f = \frac{2\mathscr{F}^f C_{1111}^s}{(\sigma_{11}^m)^2 h^f} \quad \text{and} \quad \mathscr{F}_*^s = \frac{2\mathscr{F}^s C_{1111}^s}{(\sigma_{11}^m)^2 h^f}. \tag{45}$$

The argument that the change of the total energy should not be positive at the onset of cracking, that is, $\Delta E \leqslant 0$ (Thouless, 1990), provides the critical condition for the formation of a single crack. Eq. (44) implies that the critical condition can be obtained as a function of $\mathscr{F}_*^f$, $\mathscr{F}_*^f$, h^f and h^s. The numerical results will be dealt with in part II (Lee et al., in preparation).

5.2. Critical condition for periodic cracking

The foregoing procedure, used to obtain the critical condition for the formation of a single crack, can also be used to obtain the critical condition for the formation of a periodic array of cracks, such as that as shown in Fig. 2(b). The elastic energy per unit interface area released by the crack formation is written as

$$\Delta \mathscr{E}^{el} = \frac{1}{2\lambda}\sigma_{1i}^m \int_0^{h^f} \delta_i(x_2)\,\mathrm{d}x_2 = \frac{(\sigma_{11}^m h^f)^2}{2C_{1111}^s \lambda} \mathscr{G}_*^{pc}\left(\frac{h^s}{h^f}, \frac{\lambda}{h^f}; \boldsymbol{\alpha}, \boldsymbol{\beta}\right). \tag{46}$$

Here $\mathscr{G}_*^{pc}$ is the non-dimensionalized energy release rate for a crack of the periodic array. The fracture energy per unit interface area is expressed as

$$\Delta \mathscr{E}^{fr} = \frac{1}{\lambda}(\mathscr{F}^f h^f + \mathscr{F}^s h^s). \tag{47}$$

Therefore, the total change of the energy per unit interface area becomes

$$\Delta\mathscr{E} = \frac{(\sigma_{11}^{m} h^{f})^{2}}{2C_{1111}^{s}\lambda}\left[\mathscr{F}_{*}^{f} + \mathscr{F}_{*}^{s}\frac{h^{s}}{h^{f}} - \mathscr{G}_{*}^{pc}\left(\frac{h^{s}}{h^{f}}, \frac{\lambda}{h^{f}}; \boldsymbol{\alpha}, \boldsymbol{\beta}\right)\right]. \tag{48}$$

Again, the condition $\Delta\mathscr{E} \leqslant 0$ provides the critical condition for the simultaneous formation of periodic cracks. Based on the formulation given in this paper (Part I), the numerical calculations for vertical cracking in an $In_xGa_{1-x}As$ epitaxial film on an InP substrate will be dealt with in a companion paper (Part II).

6. Summary

A vertical crack and a periodic array of vertical cracks in tensile-strained epitaxial film on a substrate are analyzed by using Stroh formalism, in which the film and the substrate have different anisotropic elastic constants. The solution for a dislocation in an anisotropic trimaterial is used as a Green function, and the cracks are modeled as the continuous distributions of dislocations, which yield the singular integral equations of Cauchy-type. The Gauss–Chebyshev quadrature formula is used to solve the singular integral equations numerically. Energy arguments yield the critical condition for crack formation, at which cracks are energetically favorable configurations, in terms of the ratio of the penetration depth into the substrate to the film thickness, the ratio of the spacing of the periodic cracks to the film thickness, and the generalized Dundurs parameters between the film and substrate materials. The numerical calculations for vertical cracking in an $In_xGa_{1-x}As$ epitaxial film on an InP substrate will be dealt with in a companion paper (Part II).

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